Gyula Tasi

List of Publications by Year
in descending order

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52	838	516215 16	525886 27
papers	citations	h-index	g-index

54	54	54	773
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Definitive thermochemistry and kinetics of the interconversions among conformers of nâ€butane and nâ€pentane. Journal of Computational Chemistry, 2018, 39, 424-437.	1.5	2
2	Comment on â€œCausation or only correlation? Application of causal inference graphs for evaluating causality in nano-QSAR modelsâ€•by N. Sizochenko, A. Gajewicz, J. Leszczynski and T. Puzyn, Nanoscale, 2016, 8, 7203. Nanoscale, 2018, 10, 20863-20866.	2.8	3
3	SYVA: A program to analyze symmetry of molecules based on vector algebra. Computer Physics Communications, 2017, 215, 156-164.	3.0	10
4	Enthalpy Differences of then-Pentane Conformers. Journal of Chemical Theory and Computation, 2016, 12, 2679-2688.	2.3	9
5	First-order chemical reaction networks I: theoretical considerations. Journal of Mathematical Chemistry, 2016, 54, 1863-1878.	0.7	5
6	Simple algebraic solutions to the kinetic problems of triangle, quadrangle and pentangle reactions. Journal of Mathematical Chemistry, 2016, 54, 85-99.	0.7	9
7	Vector algebra and molecular symmetry: a tribute to Professor Josiah Willard Gibbs. Journal of Mathematical Chemistry, 2013, 51, 2187-2195.	0.7	2
8	Benchmarking Experimental and Computational Thermochemical Data: A Case Study of the Butane Conformers. Journal of Chemical Theory and Computation, 2012, 8, 479-486.	2.3	13
9	High-Accuracy Theoretical Thermochemistry of Atmospherically Important Sulfur-Containing Molecules. Journal of Physical Chemistry A, 2011, 115, 7823-7833.	1.1	36
10	Comments on â€œShape-selective diisopropylation of naphthalene in H-mordenite: Myth or reality?â€• Journal of Catalysis, 2011, 279, 229-230.	3.1	1
11	Analytical and numerical computation of error propagation of model parameters. Journal of Mathematical Chemistry, 2011, 49, 1322-1329.	0.7	4
12	Similarity analysis of the conformational potential energy surface of n-pentane. Computational and Theoretical Chemistry, 2011, 963, 378-383.	1.1	9
13	Comment on â€œEnthalpy Difference between Conformations of Normal Alkanes: Raman Spectroscopy Study of n-Pentane and n-Butaneâ€• Journal of Physical Chemistry A, 2010, 114, 6728-6728.	1.1	4
14	High-Accuracy Theoretical Study on the Thermochemistry of Several Formaldehyde Derivatives. Journal of Physical Chemistry A, 2010, 114, 13213-13221.	1.1	19
15	Adiabatic Jacobi corrections on the vibrational energy levels of H2+ isotopologues. Journal of Chemical Physics, 2009, 130, 134314.	1.2	14
16	Energy decomposition based on the extended virial theorem: Hartreeâ€“Fock and secondâ€•order MÃ¸llerâ€“Plesset results. International Journal of Quantum Chemistry, 2009, 109, 2599-2605.	1.0	4
17	Proton affinity and enthalpy of formation of formaldehyde. International Journal of Quantum Chemistry, 2009, 109, 2393-2409.	1.0	33
18	The effect of electron correlation on the conformational space of melatonin. Journal of Computational Chemistry, 2008, 29, 1466-1471.	1.5	6

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19	Preparation of monodispersed Pt nanoparticles in MCM-41, catalytic applications. Catalysis Communications, 2008, 9, 762-768.	1.6	15
20	Hartreeâ€“Fock-limit energies and structures with a few dozen distributed Gaussians. Chemical Physics Letters, 2007, 438, 139-143.	1.2	32
21	An extension of the virial theorem for general wave functions. Chemical Physics Letters, 2007, 449, 221-226.	1.2	3
22	The Origin of Systematic Error in the Standard Enthalpies of Formation of Hydrocarbons Computed via Atomization Schemes. ChemPhysChem, 2006, 7, 1664-1667.	1.0	45
23	Catalytic detoxification of C2-chlorohydrocarbons over iron-containing oxide and zeolite catalysts. Colloids and Surfaces A: Physicochemical and Engineering Aspects, 2005, 265, 171-177.	2.3	41
24	Infrared spectroscopy studies of cyclohexene hydrogenation and dehydrogenation catalyzed by platinum nanoparticles supported on mesoporous silicate (SBA-15). Part 1: The role of particle size of Pt nanocrystals supported on SBA-15 silicate. Catalysis Letters, 2005, 101, 159-167.	1.4	13
25	Semispectroscopic and Quantitative Structureâ^'Property Relationship Estimates of the Equilibrium and Vibrationally Averaged Structure and Dipole Moment of 1-Buten-3-yne. Journal of Physical Chemistry A, 2005, 109, 4824-4828.	1.1	4
26	Molecular Shape, Dimensions, and Shape Selective Catalysis. ChemInform, 2004, 35, no.	0.1	0
27	Conformational analysis of melatonin at Hartreeâ€“Fock ab initio level. Computational and Theoretical Chemistry, 2003, 640, 69-77.	1.5	13
28	Conformational analysis of substituted (E)-4-phenylbut-3-en-2-ones. Computational and Theoretical Chemistry, 2003, 666-667, 131-134.	1.5	1
29	The stereochemistry of the chemical expression of darkness. Computational and Theoretical Chemistry, 2003, 666-667, 515-520.	1.5	5
30	Molecular shape, dimensions, and shape selective catalysis. Computational and Theoretical Chemistry, 2003, 666-667, 69-77.	1.5	16
31	1,5-Hydride shift in Wolff-Kishner reduction of (20R)-3Î²,20, 26-trihydroxy-27-norcholest-5-en-22-one: synthetic, quantum chemical, and NMR studies. Steroids, 2002, 67, 31-38.	0.8	12
32	Positional Isomerization of Dialkylnaphthalenes:Â A Comprehensive Interpretation of the Selective Formation of 2,6-DIPN over HM Zeolite. Journal of Physical Chemistry A, 2001, 105, 6513-6518.	1.1	27
33	Shape-Selective Alkylation of Isopropylnaphthalene over HM Zeolite. A Theoretical Study. Reaction Kinetics and Catalysis Letters, 2001, 74, 317-322.	0.6	11
34	Quantum algebraicâ€“combinatoric study of the conformational properties of n-alkanes. II. Journal of Mathematical Chemistry, 2000, 27, 191-199.	0.7	21
35	Molecular Electrostatics, Energetics, and Dynamics of the Alkylation of Naphthalene:Â Positional Isomerization of Monoalkylnaphthalenes at Hartreeâ^'Fock and Correlated Levels with BSSE Corrections. Journal of Physical Chemistry A, 2000, 104, 1337-1345.	1.1	13
36	Quantum algebraicâ€“combinatoric study of the conformational properties of (n)â€alkanes. I. Journal of Mathematical Chemistry, 1999, 25, 55-64.	0.7	17

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37	Generation, Characterization, and Transformations of Unsaturated Carbenium Ions in Zeolites. Chemical Reviews, 1999, 99, 2085-2114.	23.0	131
38	Generation Characterization, and Transformations of Unsaturated Carbenium Ions in Zeolites. (Chem.) Tj ETQq0 0 0 rgBT /Overlock 10 T	23.0	9
39	MEP maps as useful tools for prediction of selectivity of alkylations of fused N-heteroaromatics. Computational and Theoretical Chemistry, 1998, 455, 191-198.	1.5	5
40	Enumeration of the Conformers of Unbranched Aliphatic Alkanes. Journal of Physical Chemistry A, 1998, 102, 7698-7703.	1.1	45
41	Scaled Effective One-Electron Method Based on G2 Theory:â€‰ Results for Aliphatic Alkane Molecules. Journal of Chemical Information and Computer Sciences, 1998, 38, 632-638.	2.8	20
42	Analysis of Permanent Electric Dipole Moments of Aliphatic Hydrocarbon Molecules. 2. DFT Results. Journal of Chemical Information and Computer Sciences, 1998, 38, 313-316.	2.8	6
43	Analysis of permanent electric dipole moments of aliphatic hydrocarbon molecules. Computational and Theoretical Chemistry, 1997, 401, 21-27.	1.5	15
44	A new program for effective one-electron (EHMO-ASED) calculations. Computers & Chemistry, 1997, 21, 319-325.	1.2	6
45	Investigation of the surface reactions of CCl4 on zeolites studied by IR and MAS NMR spectroscopy. Colloids and Surfaces A: Physicochemical and Engineering Aspects, 1995, 101, 199-206.	2.3	19
46	Hydrogen bonding interactions of Î±-phenylcinnamic acid isomers in the liquid phase studied by IR and NMR spectroscopies and computational methods. Journal of Molecular Structure, 1995, 348, 57-60.	1.8	20
47	Spectra of carbanions formed from allyl cyanide during isomerization in zeolite NaY-FAU with strong basic sites. Journal of Molecular Structure, 1995, 348, 345-348.	1.8	4
48	Adsorption-induced Fermi resonance among the vibrations of intermediates formed on BrÃ¸nsted acidic zeolites. Spectroscopic and theoretical description. Journal of Molecular Structure, 1995, 351, 1-5.	1.8	7
49	Using molecular electrostatic potential maps for similarity studies. Topics in Current Chemistry, 1995, , 45-71.	4.0	25
50	Calculation of electrostatic potential maps and atomic charges for large molecules. Journal of Chemical Information and Computer Sciences, 1993, 33, 296-299.	2.8	28
51	Representation of molecules by atomic charges: A new population analysis. Journal of Computational Chemistry, 1992, 13, 371-379.	1.5	13
52	Formation of Carbocations from C6 Compounds in Zeolites. Studies in Surface Science and Catalysis, 1989, , 355-364.	1.5	12